

FIG. 1

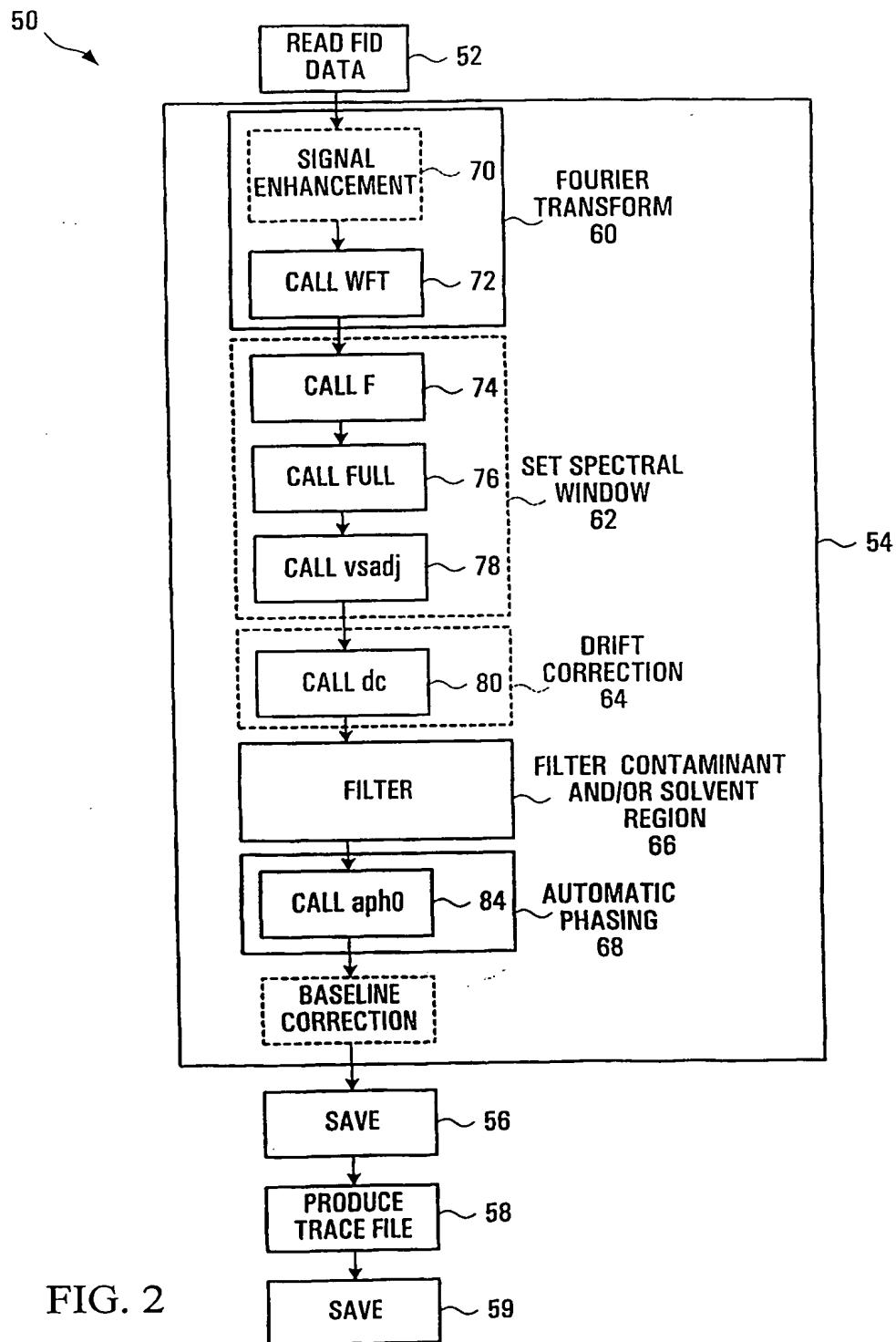
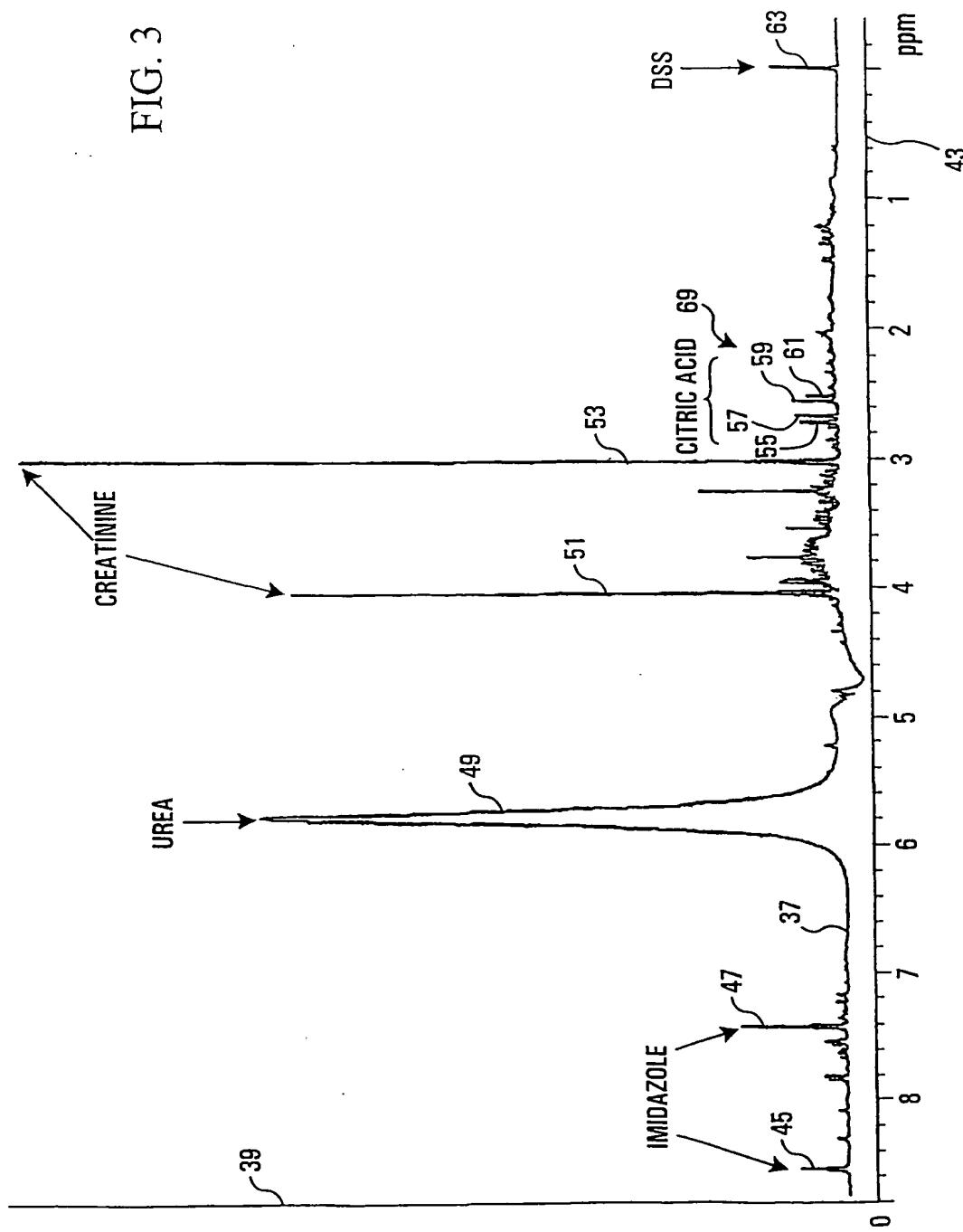


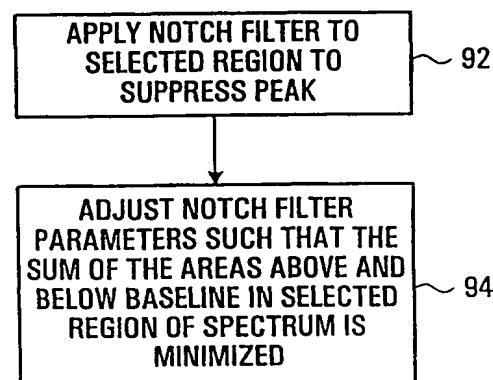
FIG. 2

FIG. 3



66

**FILTER SELECTED REGION**



**FIG. 4**

PROCESS FOR IDENTIFYING  
COMPOUNDS FROM A TEST  
SPECTRUM

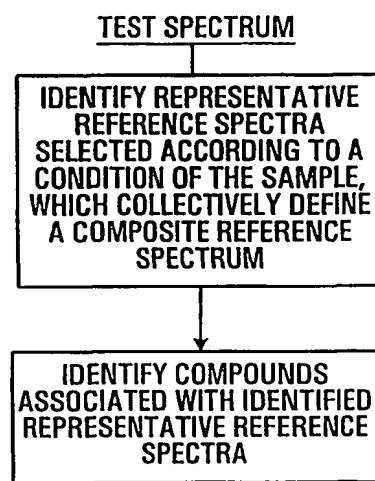
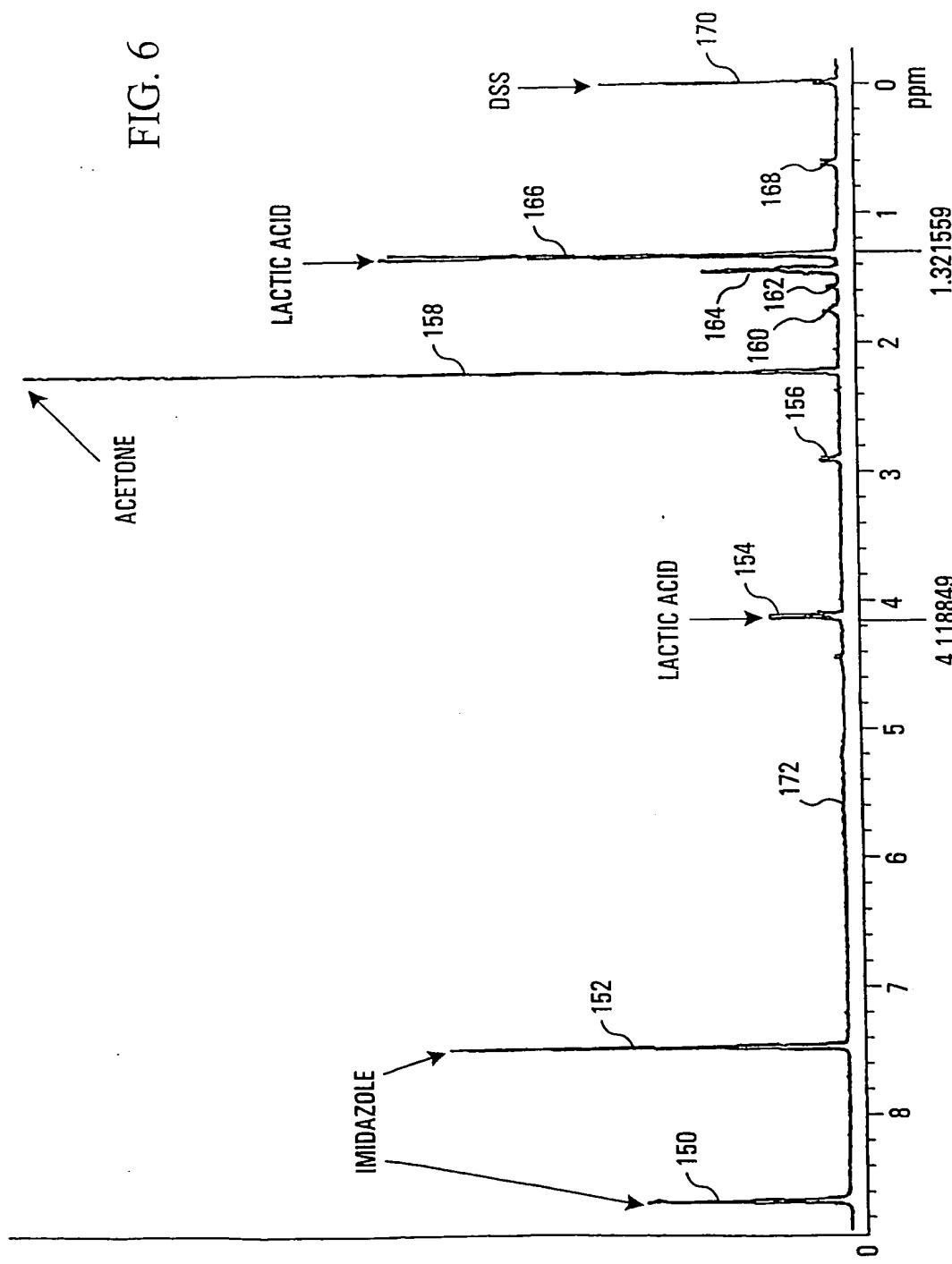


FIG. 5

FIG. 6



**REAL SPECTRAL DATA - pH=5.10**

```
<?xml version="1.0"?>
<!--compoundDB version="2.0"-->
<compound>
  <name>LacticAcid</name>
  <molecularWeight>90.08</molecularWeight>
```

```
<experiment>
  <pH>5.1</pH>
  <temperatureKelvin>298.150000</temperatureKelvin>
  <DSSRatio>0.533668</DSSRatio>
  <concentration>4.308710</concentration>
  <timestamp>Sept 5 2001</timestamp>
  <sourceFID>lacticacid.fid</sourceFID>
  <magnetMHz>400.120773</magnetMHz>
  <spectralWidthHz>6006.006006</spectralWidthHz>
</experiment>
```

```
<cluster>
  210-><protonNumber>3</protonNumber>
  212-><quantification>1</quantification>
  <subCluster>
    214-><lorentzianWidthAdjust>2.893258</lorentzianWidthAdjust>
    <peak>
      220-><offsetCenterHz>-3.455480</offsetCenterHz>
      222-><height>0.988680</height>
      224-><protonRatio>1.491461</protonRatio>
    </peak>
    <peak>
      226-><offsetCenterHz>3.455480</offsetCenterHz>
      228-><height>1.0000000</height>
      230-><protonRatio>1.508539</protonRatio>
    </peak>
  </subCluster>
</cluster>
```

206  
202  
204  
216  
218  
FIG. 7A

```
<cluster>
<protonNumber> 1 </protonNumber>
<quantification> 0 </quantification>
<subCluster>
<centerPPM> 4.118849 </centerPPM>
<lorentzianWidthAdjust> 13.441432 <lorentzianWidthAdjust>
<peak>
<offsetCenterHz> -10.366999 </offsetCenterHz>
<height> 0.057244 </height>
<protonRatio> 0.130861 </protonRatio>
</peak>
<peak>
<offsetCenterHz> -3.43221144 </offsetCenterHz>
<height> 0.164751 </height>
<protonRatio> 0.376629 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 3.487744 </offsetCenterHz>
<height> 0.161840 </height>
<protonRatio> 0.369975 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 10.366999 </offsetCenterHz>
<height> 0.053601 </height>
<protonRatio> 0.122535 </protonRatio>
</peak>
</subCluster>
</cluster>
</compound>
```

208

204

FIG. 7B

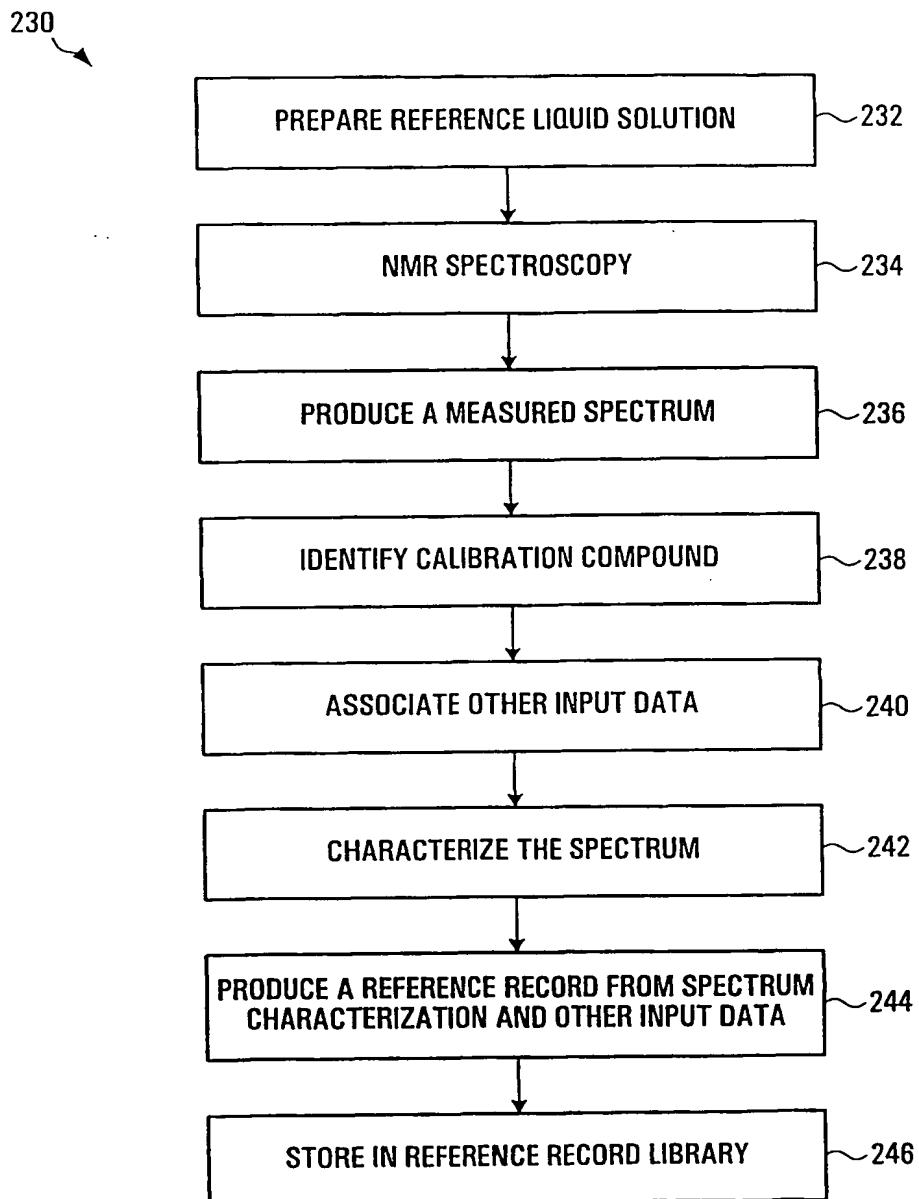


FIG. 8

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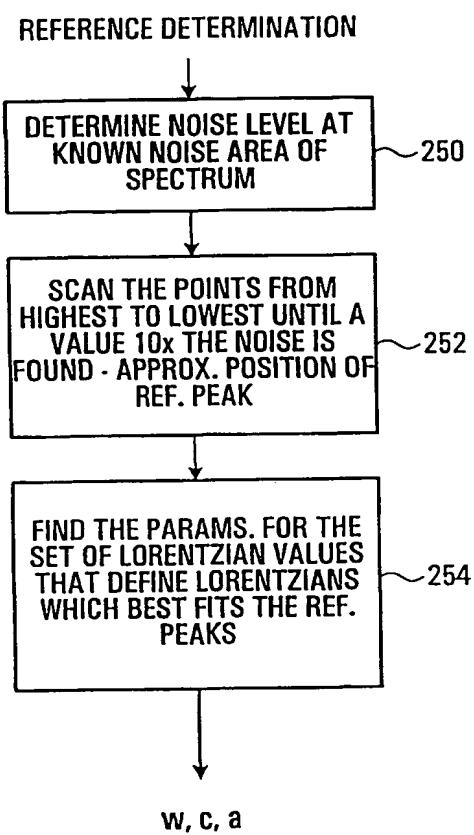


FIG. 9

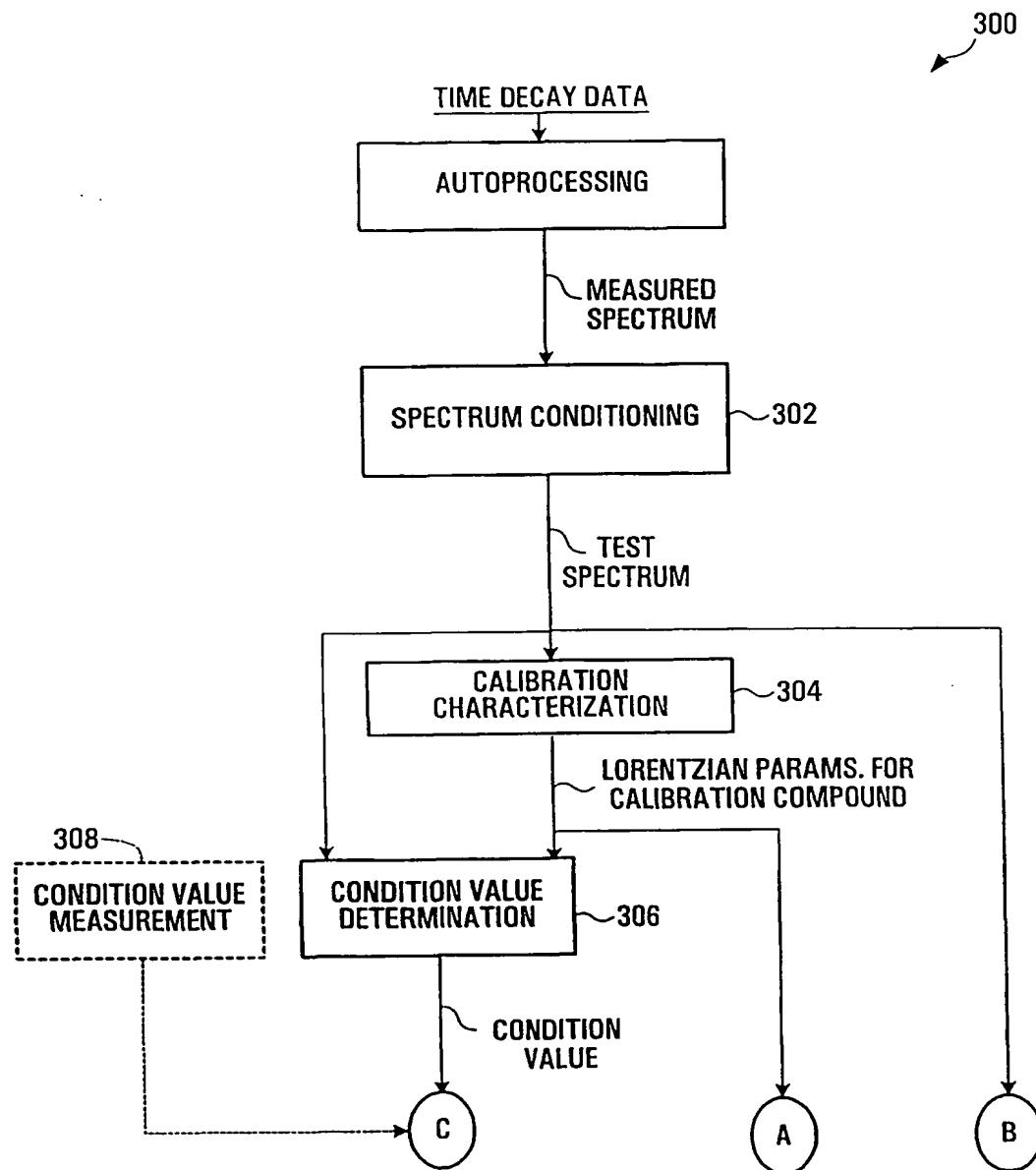


FIG. 10A

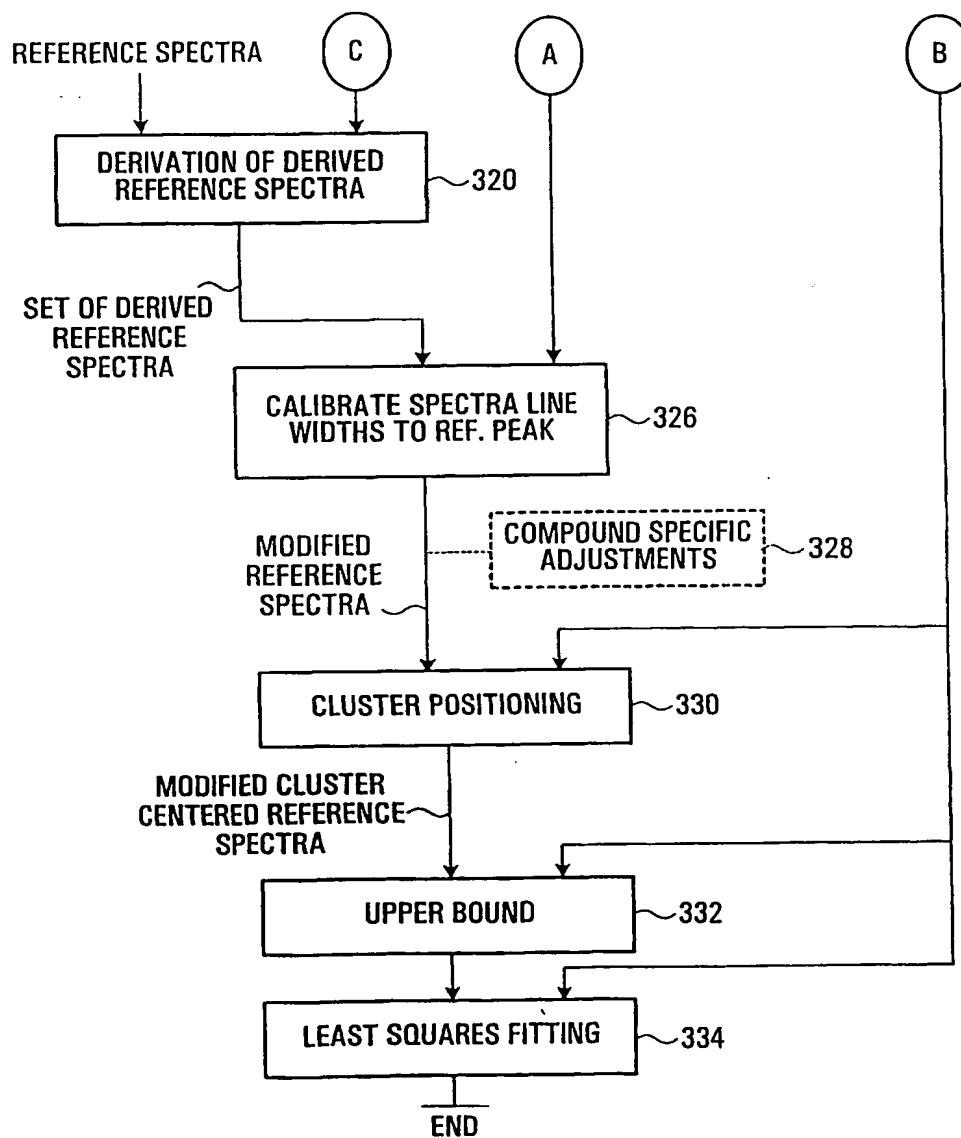


FIG. 10B

CONDITION VALUE DETERMINATION

310

(x, y)                            w, c, a

SCAN POINTS FROM LEFT SIDE IN  
PREDEF. WINDOW ABOUT  
EXPECTED pH REFERENCE PEAK  
UNTIL A POINT HAVING AN  
AMPLITUDE > pH REFERENCE  
PEAK FOUND

~312

FIND THE PARAMETERS FOR  
THE SET OF LORENTZIAN  
VALUES WHICH DEFINE  
LORENTZIAN WHICH BEST  
FITS THE pH REFERENCE  
PEAK

~314

MODIFIED TITRATION  
EQUATION WITH  
PARAMETERS DETERMINED  
BY SOLVENT

~316

pH VALUE

RETURN

FIG. 11

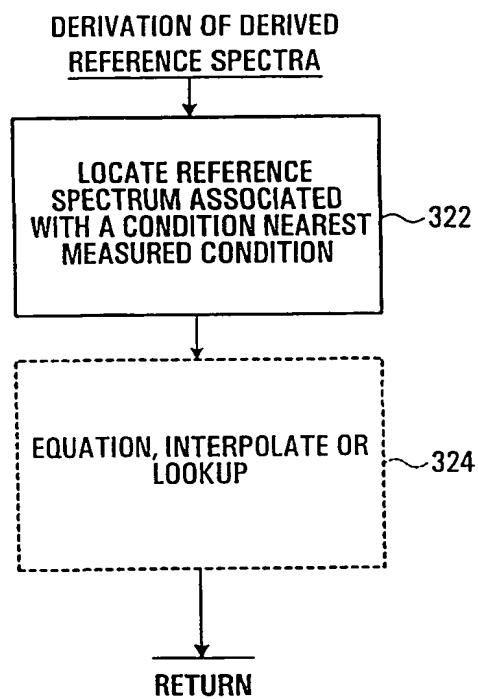


FIG. 12

## Real Spectral Data · pH=5.45

```
<?xml version="1.0"?>
<!-- compoundDB version="2.0" -->
<compound>
<name>LacticAcid</name>
<molecularWeight>90.08</molecularWeight>

<experiment>
<pH>5.45</pH>
<temperatureKelvin>298.150000</temperatureKelvin>
<DSSRatio>0.533668</DSSRatio>
<concentration>4.308710</concentration>
<timestamp>Sept 5 2001</timestamp>
<sourceFID>lacticacid.fid</sourceFID>
<magnetMHz>400.120699</magnetMHz>
<spectralWidthHz>6006.006006</spectralWidthHz>
</experiment>

<cluster>
<protonNumber>3</protonNumber>
<quantification>1</quantification>
<subCluster>
<centerPPM>1.318770</centerPPM>
<lorentzianWidthAdjust>1.562004</lorentzianWidthAdjust>
<peak>
<offsetCenterHz>-3.453329</offsetCenterHz>
<height>0.983656</height>
<protonRatio>1.487641</protonRatio>
</peak>
<peak>
<offsetCenterHz>3.453329</offsetCenterHz>
<height>1.000000</height>
<protonRatio>1.512359</protonRatio>
</peak>
</subCluster>
</cluster>
```

FIG. 13A

```
<cluster>
<protonNumber> 1 </protonNumber>
<quantification> 0 </quantification>
<subCluster>
<centerPPM> 4.110990 </centerPPM>
<lorentzianWidthAdjust> 7.044502 </lorentzianWidthAdjust>
<peak>
<offsetCenterHz> -10.371092 </offsetCenterHz>
<height> 0.054671 </height>
<protonRatio> 0.124148 </protonRatio>
</peak>
<peak>
<offsetCenterHz> -3.448909 </offsetCenterHz>
<height> 0.164509 </height>
<protonRatio> 0.373572 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 3.456819 </offsetCenterHz>
<height> 0.163879 </height>
<protonRatio> 0.372141 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 10.371092 </offsetCenterHz>
<height> 0.057309 </height>
<protonRatio> 0.130139 </protonRatio>
</peak>
</subCluster>
</cluster>
</compound>
```

FIG. 13B

**Interpolated Data - pH=5.28**

```
<?xml version="1.0"?>
<!-- compoundDB version="2.0" -->
<compound>
  <name>LacticAcid</name>
  <molecularWeight>90.08</molecularWeight>

  <experiment>
    <pH>5.45</pH>
    <temperatureKelvin>298.150000</temperatureKelvin> : copied
    <DSSRatio>0.533668</DSSRatio>
    <concentration>4.308710</concentration>
    <timestamP>Sept 5 2001</timestamP>
    <sourceFID>lacticacid.fid</sourceFID> : copied
    <magnetMHz>400.120699</magnetMHz>
    <spectralWidthHz>6006.006006</spectralWidthHz>
  </experiment>

  <cluster>
    <protonNumber>3</protonNumber>
    <quantification>1</quantification>
    <subCluster>
      <centerPPM>1.3202</centerPPM> : interpolated
      <lorentzianWidthAdjust>1.562004</lorentzianWidthAdjust>
      <peak>
        <offsetCenterHz>-3.453329</offsetCenterHz>
        <height>0.983656</height>
        <protonRatio>1.487641</protonRatio>
      </peak>
      <peak>
        <offsetCenterHz>3.453329</offsetCenterHz>
        <height>1.000000</height>
        <protonRatio>1.512359</protonRatio>
      </peak>
    </subCluster>
  </cluster>
```

FIG. 14A

```
<cluster>
<protonNumber> 1 </protonNumber>
<quantification> 0 </quantification>
<subCluster>
<centerPPM> 4.1149 </centerPPM> :interpolated
<lorentzianWidthAdjust> 7.044502 </lorentzianWidthAdjust>
<peak>
<offsetCenterHz> -10.371092 </offsetCenterHz>
<height> 0.054671 </height>
<protonRatio> 0.124148 </protonRatio>
</peak>
<peak>
<offsetCenterHz> -3.448909 </offsetCenterHz>
<height> 0.164509 </height>
<protonRatio> 0.373572 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 3.456819 </offsetCenterHz>
<height> 0.163879 </height>
<protonRatio> 0.372141 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 10.371092 </offsetCenterHz>
<height> 0.057309 </height>
<protonRatio> 0.130139 </protonRatio>
</peak>
</subCluster>
</cluster>
</compound>
```

FIG. 14B

### Generic Lactic Acid record

```
<?xml version="1.0"?>
<!-- compoundDB version="2.0" -->
<compound>
  <name>LacticAcid</name>
  <molecularWeight>90.08</molecularWeight>

  <experiment>
    <pH>5.45</pH>
    <temperatureKelvin>298.150000</temperatureKelvin>
    <DSSRatio>0.533668</DSSRatio>
    <concentration>4.308710</concentration>
    <timestamP>Sept 5 2001</timestamP>
    <sourceFID>lacticacid.fid</sourceFID>
    <magnetMHz>400.120699</magnetMHz>
    <spectralWidthHz>6006.006006</spectralWidthHz>
  </experiment>

  <cluster>
    <protonNumber>3</protonNumber>
    <quantification>1</quantification>
    <subCluster>
      <centerPPM>y=m1(pH)+b1</centerPPM>
      <lorentzianWidthAdjust>1.562004</lorentzianWidthAdjust>
      <peak>
        <offsetCenterHz>-3.453329</offsetCenterHz>
        <height>0.983656</height>
        <protonRatio>1.487641</protonRatio>
      </peak>
      <peak>
        <offsetCenterHz>3.453329</offsetCenterHz>
        <height>1.000000</height>
        <protonRatio>1.512359</protonRatio>
      </peak>
    </subCluster>
  </cluster>
```

FIG. 15A

```
<cluster>
<protonNumber> 1 </protonNumber>
<quantification> 0 </quantification>
<subCluster>
<centerPPM> y=m2(pH)+b2 </centerPPM>
<lorentzianWidthAdjust> 7.044502 </lorentzianWidthAdjust>
<peak>
<offsetCenterHz> -10.371092 </offsetCenterHz>
<height> 0.054671 </height>
<protonRatio> 0.124148 </protonRatio>
</peak>
<peak>
<offsetCenterHz> -3.448909 </offsetCenterHz>
<height> 0.164509 </height>
<protonRatio> 0.373572 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 3.456819 </offsetCenterHz>
<height> 0.163879 </height>
<protonRatio> 0.372141 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 10.371092 </offsetCenterHz>
<height> 0.057309 </height>
<protonRatio> 0.130139 </protonRatio>
</peak>
</subCluster>
</cluster>
</compound>
```

FIG. 15B

**Generic Lactic Acid record with Lookup Table link**

```
<?xml version="1.0"?>
<!-- compoundDB version="2.0" -->
<b>compound</b>
<name>LacticAcid</name>
<molecularWeight>90.08</molecularWeight>

<b>experiment</b>
<pH>5.45</pH>
<temperatureKelvin>298.150000</temperatureKelvin>
<DSSRatio>0.533668</DSSRatio>
<concentration>4.308710</concentration>
<timestamp>Sept 5 2001</timestamp>
<sourceFID>lacticacid.fid</sourceFID>
<magnetMHz>400.120699</magnetMHz>
<spectralWidthHz>6006.006006</spectralWidthHz>
</experiment>

<b>cluster</b>
<protonNumber>3</protonNumber>
<quantification>1</quantification>
<subCluster>
<centerPPM>LOOKUP TABLE LINK1</centerPPM>
<lorentzianWidthAdjust>1.562004</lorentzianWidthAdjust>
<b>peak</b>
<offsetCenterHz>-3.453329</offsetCenterHz>
<height>0.983656</height>
<protonRatio>1.487641</protonRatio>
</peak>
<b>peak</b>
<offsetCenterHz>3.453329</offsetCenterHz>
<height>1.000000</height>
<protonRatio>1.512359</protonRatio>
</peak>
</subCluster>
</cluster>
```

FIG. 16A

```
<cluster>
<protonNumber> 1 </protonNumber>
<quantification> 0 </quantification>
<subCluster>
<centerPPM> LOOKUP TABLE LINK2 </centerPPM>
<lorentzianWidthAdjust> 7.044502 </lorentzianWidthAdjust>
<peak>
<offsetCenterHz> -10.371092 </offsetCenterHz>
<height> 0.054671 </height>
<protonRatio> 0.124148 </protonRatio>
</peak>
<peak>
<offsetCenterHz> -3.448909 </offsetCenterHz>
<height> 0.164509 </height>
<protonRatio> 0.373572 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 3.456819 </offsetCenterHz>
<height> 0.163879 </height>
<protonRatio> 0.372141 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 10.371092 </offsetCenterHz>
<height> 0.057309 </height>
<protonRatio> 0.130139 </protonRatio>
</peak>
</subCluster>
</cluster>
</compound>
```

FIG. 16B

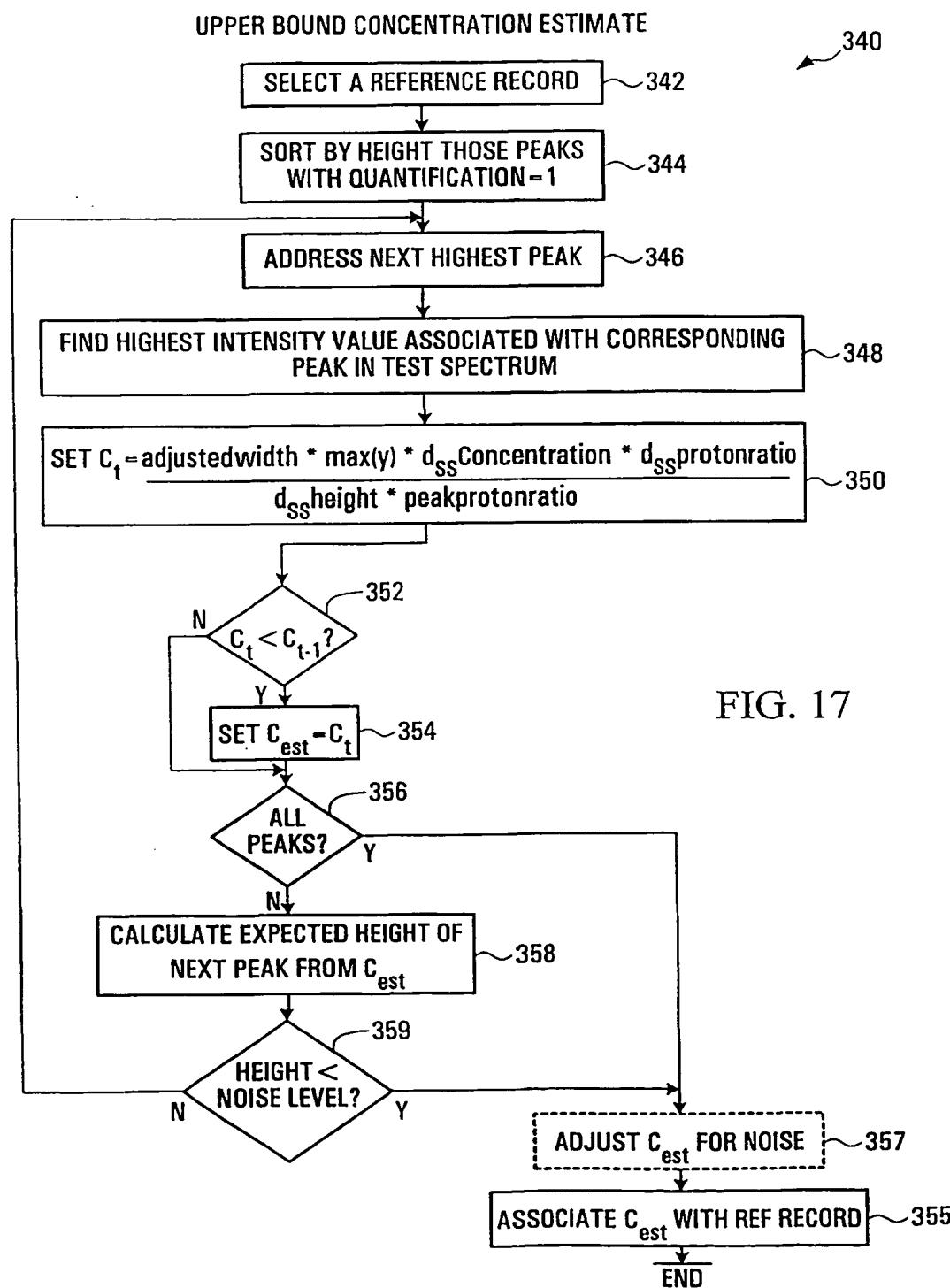


FIG. 17

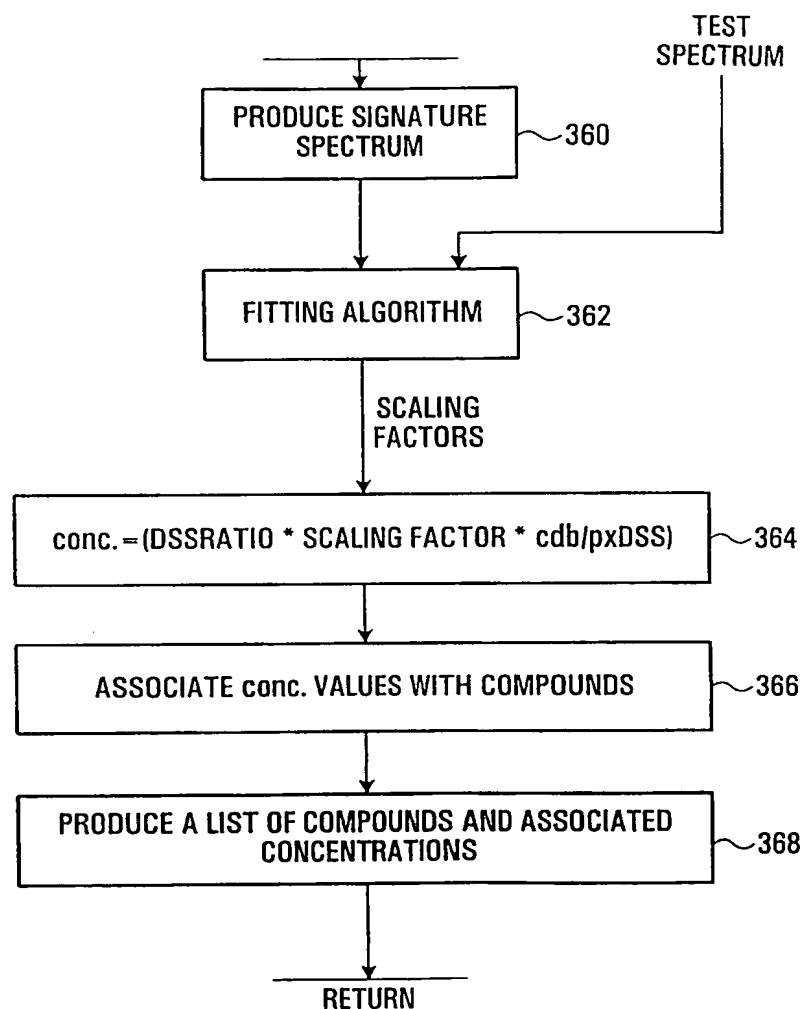


FIG. 18